

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062023\
 Data File : BP015631.D
 Acq On : 20 Jun 2023 20:26
 Operator : MA/JU
 Sample : 03080-20
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 DCFQ5

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0.1 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BP015631.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.405	33	37	45	rVB	28782	43156	0.87%	0.083%
2	3.711	86	89	93	rBV	8469	10297	0.21%	0.020%
3	3.852	111	113	127	rBV	191503	328462	6.60%	0.631%
4	3.952	127	130	136	rVB	34687	46257	0.93%	0.089%
5	4.075	147	151	157	rVB2	15805	25114	0.50%	0.048%
6	4.175	165	168	172	rVB4	5487	7476	0.15%	0.014%
7	4.558	231	233	240	rVB8	4687	7925	0.16%	0.015%
8	4.758	262	267	274	rVB8	5015	10028	0.20%	0.019%
9	5.240	347	349	357	rVB9	4637	8850	0.18%	0.017%
10	6.299	524	529	535	rBV3	7871	16166	0.32%	0.031%
11	6.734	597	603	609	rVB4	22449	40189	0.81%	0.077%
12	7.040	651	655	659	rBV7	4124	6711	0.13%	0.013%
13	7.093	661	664	670	rVB6	4923	9540	0.19%	0.018%
14	7.246	683	690	706	rBV	598484	1016149	20.41%	1.954%
15	7.405	711	717	727	rVB	450747	713100	14.32%	1.371%
16	7.505	729	734	738	rVB7	7053	10248	0.21%	0.020%
17	7.611	745	752	762	rBV	630531	1030623	20.70%	1.981%
18	7.893	797	800	807	rVB9	3405	6647	0.13%	0.013%
19	8.081	826	832	844	rVB	437498	709529	14.25%	1.364%
20	8.805	948	955	971	rBV	664940	1150375	23.10%	2.212%
21	8.922	971	975	981	rVB7	5927	11704	0.24%	0.023%
22	9.263	1025	1033	1048	rBV	651476	1099997	22.09%	2.115%
23	9.410	1054	1058	1065	rVB5	12336	20884	0.42%	0.040%
24	9.987	1146	1156	1175	rBV	573942	1012657	20.34%	1.947%
25	10.216	1189	1195	1197	rBV7	5937	10948	0.22%	0.021%
26	10.534	1242	1249	1269	rBV	742071	1412440	28.37%	2.715%
27	10.910	1306	1313	1320	rBV	651146	1072522	21.54%	2.062%
28	11.057	1330	1338	1356	rBV	459578	964097	19.36%	1.853%
29	11.716	1443	1450	1458	rBV7	8150	18962	0.38%	0.036%
30	11.910	1478	1483	1487	rBV7	4680	10006	0.20%	0.019%
31	12.404	1560	1567	1570	rBV7	4203	6874	0.14%	0.013%
32	12.493	1575	1582	1589	rVB2	13931	24930	0.50%	0.048%
33	12.569	1589	1595	1601	rBV9	3491	6777	0.14%	0.013%
34	13.010	1665	1670	1676	rBV9	4526	8070	0.16%	0.016%
35	13.087	1678	1683	1692	rVB9	7228	16666	0.33%	0.032%
36	13.246	1703	1710	1716	rVV9	3401	7671	0.15%	0.015%

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Integrator: RTE
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 Stop Thrs : 0 Peak Location: TOP

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37	13.328	1718	1724	1731	rVB7	7206	13609	0.27%	0.026%
38	13.604	1765	1771	1778	rVB3	21469	42552	0.85%	0.082%
39	13.687	1781	1785	1787	rBV5	4661	7449	0.15%	0.014%
40	13.993	1831	1837	1840	rBV8	3571	5170	0.10%	0.010%
41	14.040	1840	1845	1851	rVV3	52250	76648	1.54%	0.147%
42	14.134	1853	1861	1876	rBV	1579854	2184255	43.87%	4.199%
43	14.240	1877	1879	1883	rVB5	5935	7056	0.14%	0.014%
44	14.422	1904	1910	1922	rBV	1751352	2609019	52.40%	5.016%
45	14.604	1937	1941	1946	rVB8	6056	10771	0.22%	0.021%
46	14.675	1947	1953	1956	rBV6	14591	23005	0.46%	0.044%
47	14.728	1956	1962	1969	rVV	1035532	1491530	29.96%	2.867%
48	14.951	1990	2000	2022	rBV	476809	1201906	24.14%	2.311%
49	15.104	2022	2026	2027	rVV4	28392	41130	0.83%	0.079%
50	15.128	2027	2030	2042	rVB6	33750	76454	1.54%	0.147%
51	15.398	2074	2076	2082	rVB7	8394	10959	0.22%	0.021%
52	15.498	2088	2093	2097	rBV6	7278	13338	0.27%	0.026%
53	15.540	2097	2100	2107	rVB6	12308	18979	0.38%	0.036%
54	15.628	2113	2115	2119	rVB5	7649	8708	0.17%	0.017%
55	15.722	2124	2131	2137	rBV	2290841	3279507	65.86%	6.305%
56	15.769	2137	2139	2148	rVV5	21781	40079	0.80%	0.077%
57	15.857	2148	2154	2168	rVV	661170	1009408	20.27%	1.941%
58	15.957	2168	2171	2177	rVB3	16649	27581	0.55%	0.053%
59	16.087	2187	2193	2201	rBV	381103	544978	10.95%	1.048%
60	16.287	2224	2227	2231	rVB6	6680	9334	0.19%	0.018%
61	16.345	2234	2237	2243	rVB8	6895	12043	0.24%	0.023%
62	16.439	2246	2253	2262	rBV8	14979	37839	0.76%	0.073%
63	16.575	2273	2276	2280	rBV6	5840	9660	0.19%	0.019%
64	16.863	2321	2325	2328	rBV6	17236	25088	0.50%	0.048%
65	17.010	2347	2350	2355	rVB5	17718	25581	0.51%	0.049%
66	17.210	2381	2384	2389	rBV5	11125	15596	0.31%	0.030%
67	17.357	2405	2409	2417	rBV5	37063	66257	1.33%	0.127%
68	17.428	2417	2421	2425	rBV6	15193	24055	0.48%	0.046%
69	17.486	2425	2431	2436	rVV	1460401	2044848	41.07%	3.931%
70	17.528	2436	2438	2441	rVV	32924	41520	0.83%	0.080%
71	17.586	2442	2448	2461	rVB	2594334	3746092	75.23%	7.202%
72	18.122	2537	2539	2543	rVB5	11126	12420	0.25%	0.024%
73	18.228	2555	2557	2562	rVB4	24936	32841	0.66%	0.063%
74	18.286	2563	2567	2571	rBV3	39567	58920	1.18%	0.113%
75	18.345	2572	2577	2586	rBV	1106830	1446063	29.04%	2.780%
76	18.622	2621	2624	2630	rBV7	21903	43668	0.88%	0.084%

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77	19.222	2723	2726	2732	rBV3	34671	52756	1.06%	0.101%
78	19.380	2751	2753	2757	rVB2	43114	53156	1.07%	0.102%
79	19.428	2758	2761	2762	rBV2	45928	46527	0.93%	0.089%
80	19.457	2762	2766	2767	rVV2	92032	119050	2.39%	0.229%
81	19.480	2767	2770	2777	rVB	122200	177716	3.57%	0.342%
82	19.563	2781	2784	2792	rBV	376254	512949	10.30%	0.986%
83	19.810	2820	2826	2834	rBV	3846818	4979205	100.00%	9.572%
84	21.098	3041	3045	3051	rVB	266663	316824	6.36%	0.609%
85	21.239	3065	3069	3077	rVB2	737629	1089213	21.88%	2.094%
86	21.569	3120	3125	3129	rVB	1706293	2253594	45.26%	4.332%
87	22.204	3230	3233	3241	rVB2	219343	367395	7.38%	0.706%
88	23.274	3411	3415	3421	rVB	631058	1015519	20.40%	1.952%
89	23.351	3425	3428	3439	rVB2	380300	817098	16.41%	1.571%
90	23.951	3523	3530	3543	rVB2	2320985	4871067	97.83%	9.364%
91	24.116	3552	3558	3568	rVB2	1016209	2154638	43.27%	4.142%
92	24.727	3656	3662	3671	rVB	838296	1891949	38.00%	3.637%

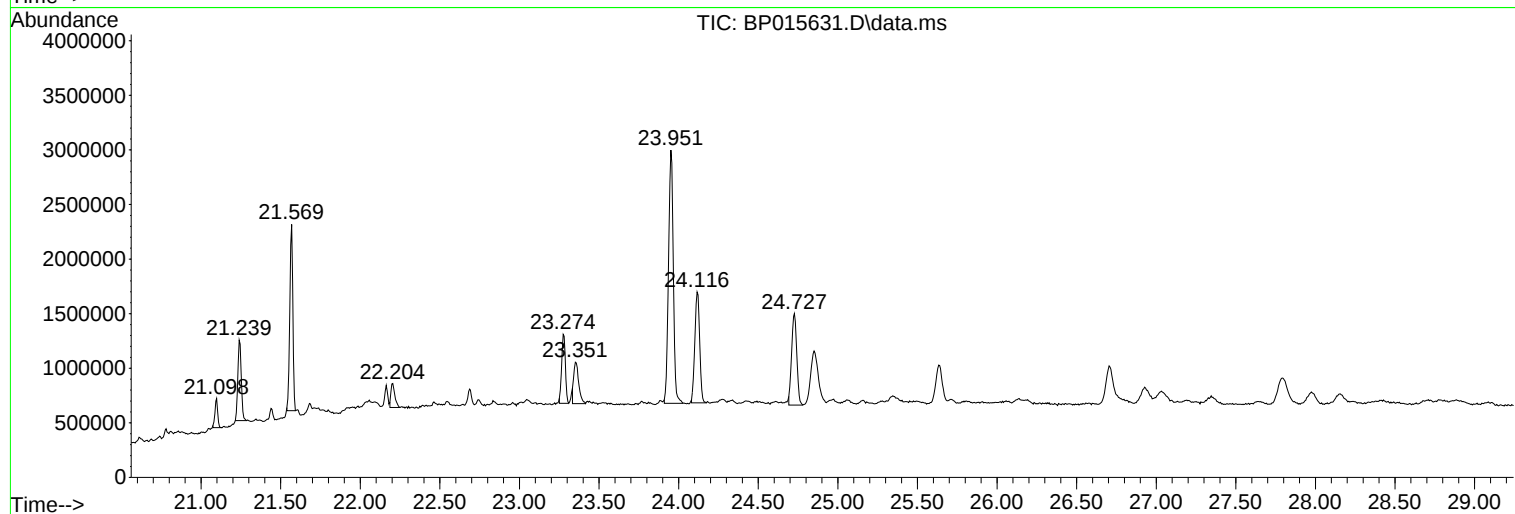
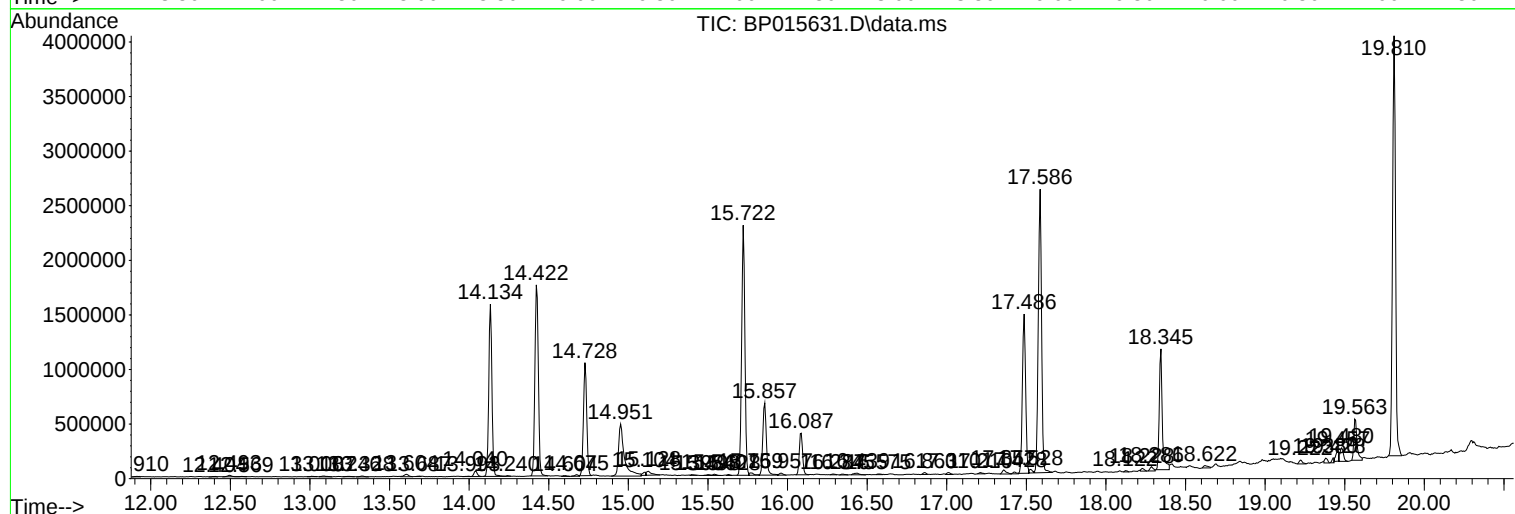
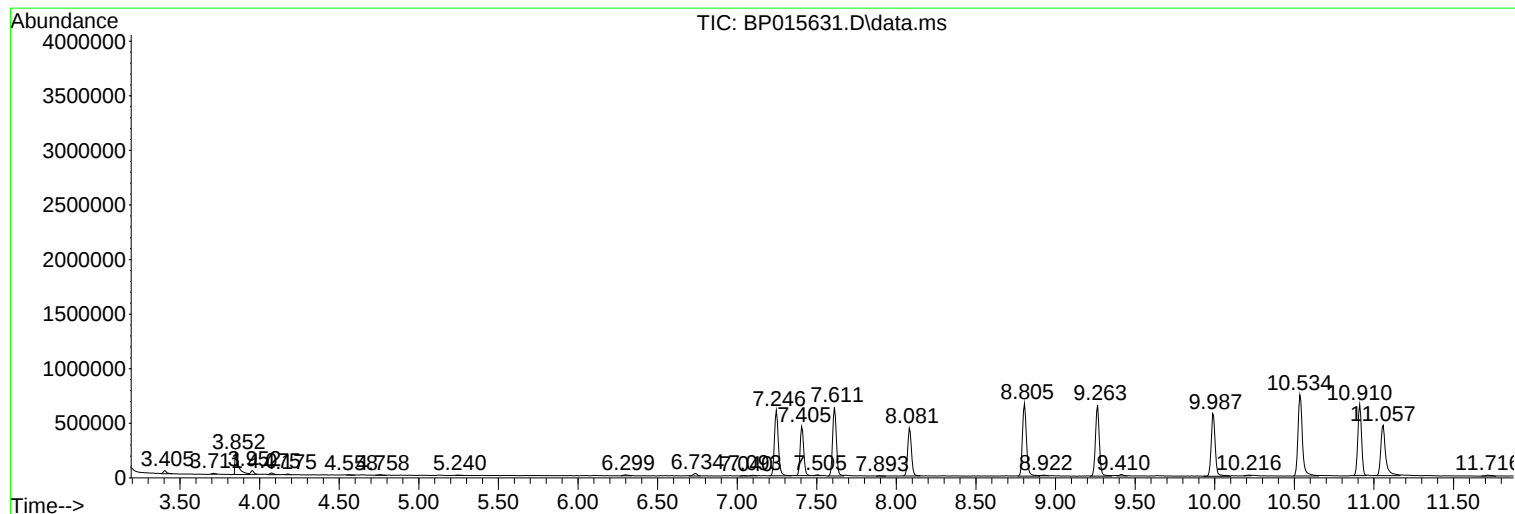
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P



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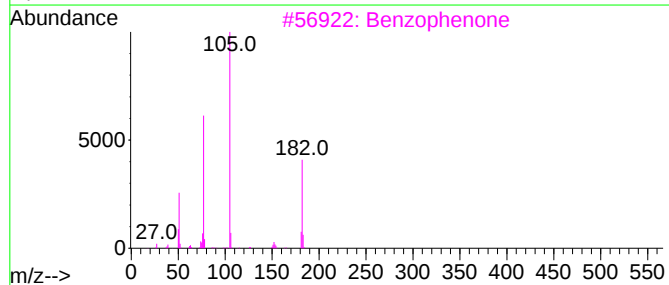
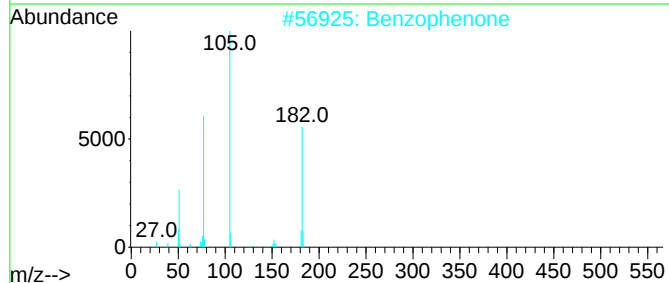
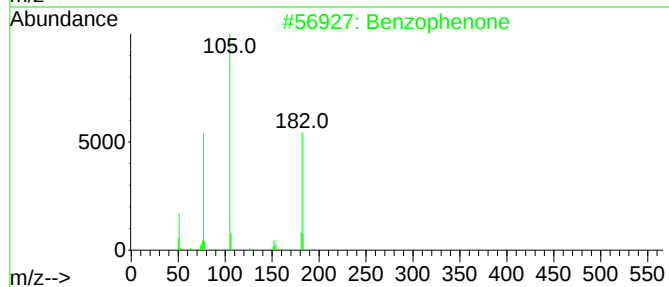
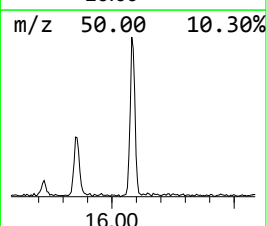
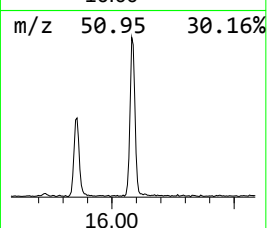
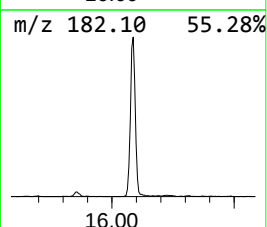
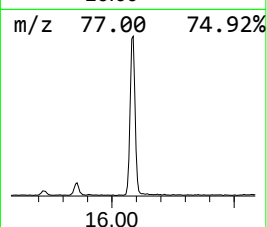
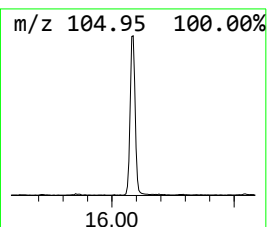
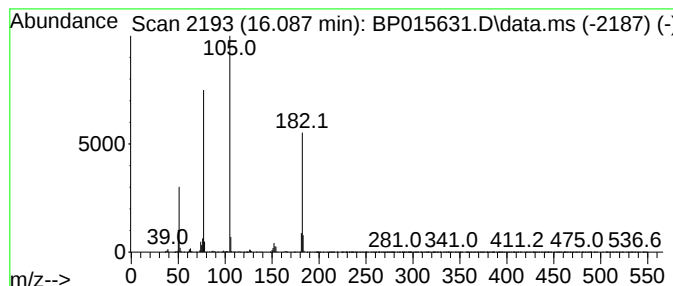
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.087	7.31 ng/ul	544978	Acenaphthene-d10	14.728

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzophenone	182	C13H10O	000119-61-9	96
3			Benzophenone	182	C13H10O	000119-61-9	96
4			Benzophenone	182	C13H10O	000119-61-9	95
5			Benzophenone	182	C13H10O	000119-61-9	91



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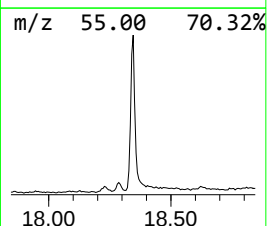
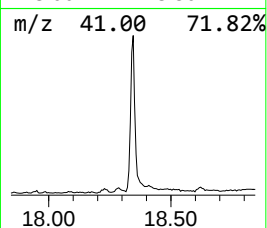
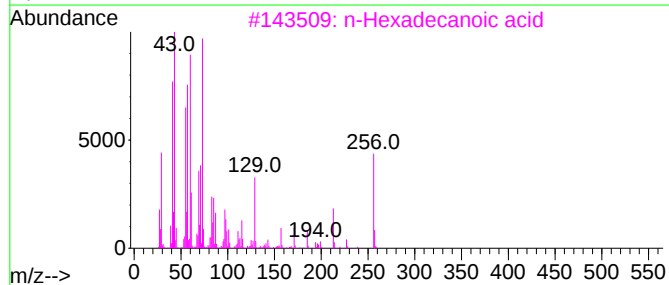
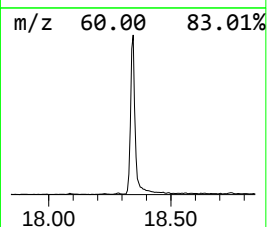
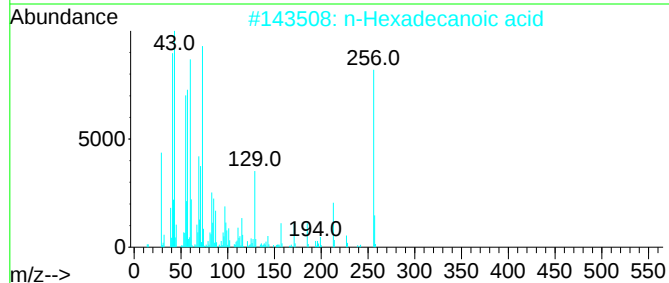
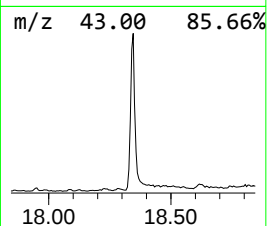
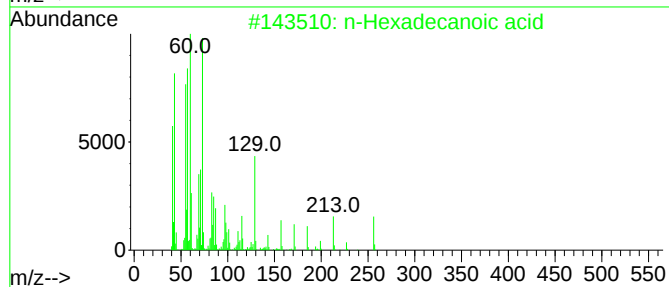
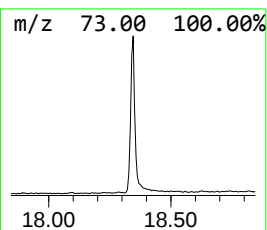
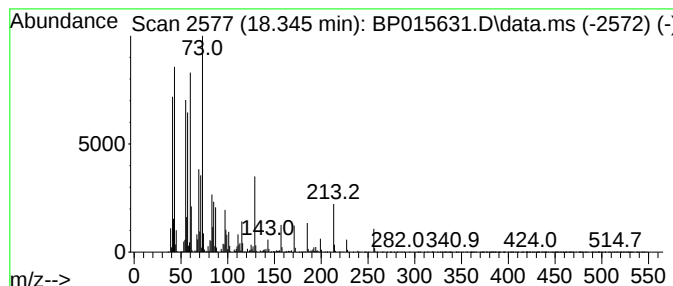
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.345	14.14 ng/ul	1446060	Phenanthrene-d10	17.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
5			Tridecanoic acid	214	C13H26O2	000638-53-9	95



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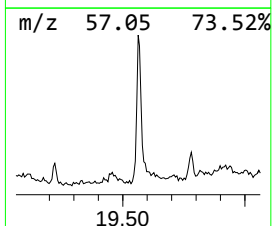
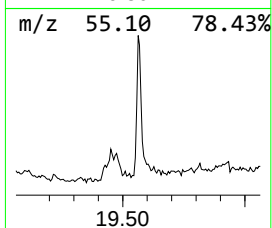
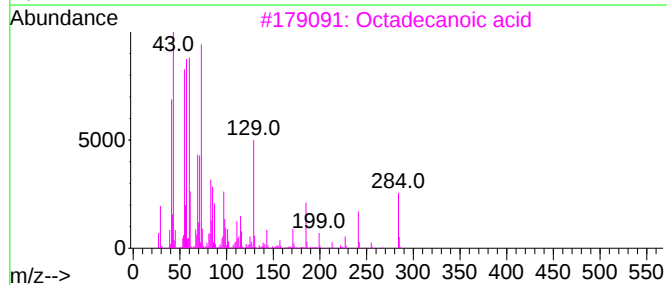
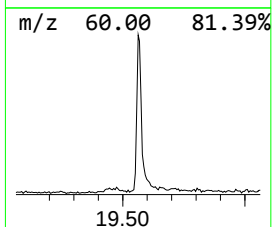
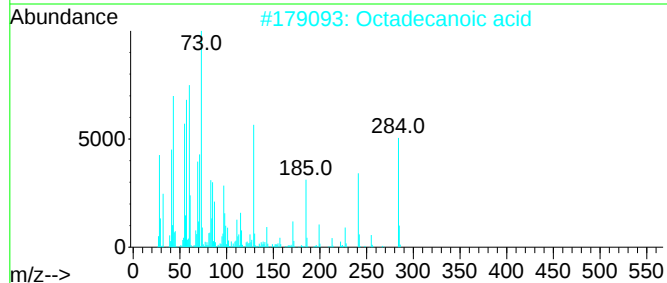
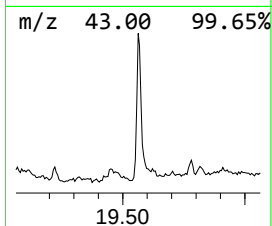
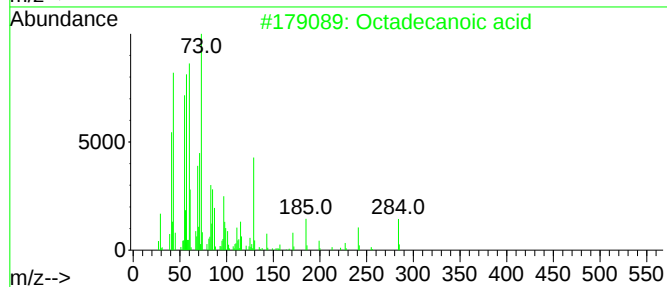
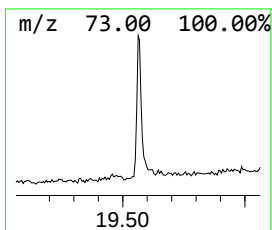
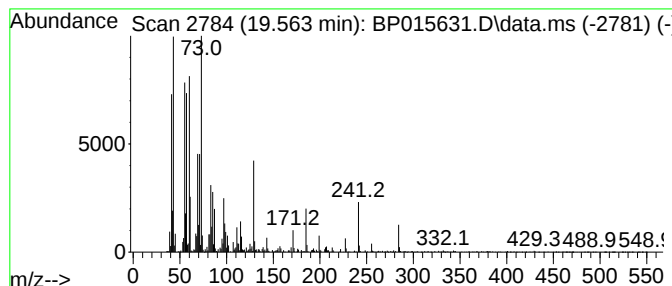
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.563	4.55 ng/ul	512949	Chrysene-d12	21.569

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Octadecanoic acid	284	C18H36O2	000057-11-4	99
3			Octadecanoic acid	284	C18H36O2	000057-11-4	99
4			Octadecanoic acid	284	C18H36O2	000057-11-4	98
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	93



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Operator : MA/JU
Sample : 03080-20
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFQ5

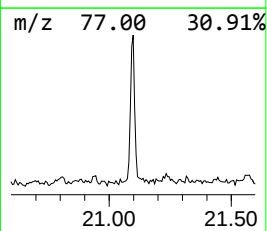
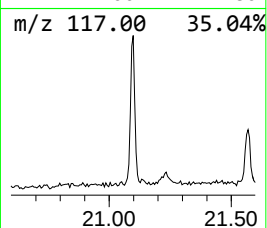
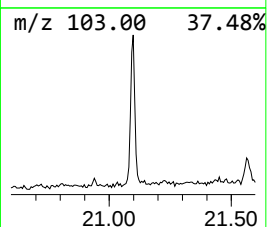
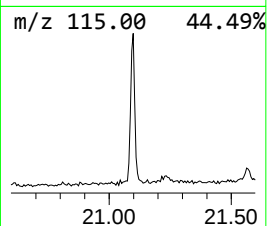
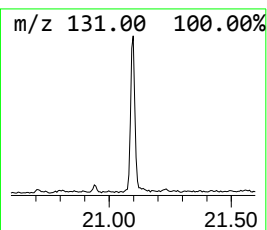
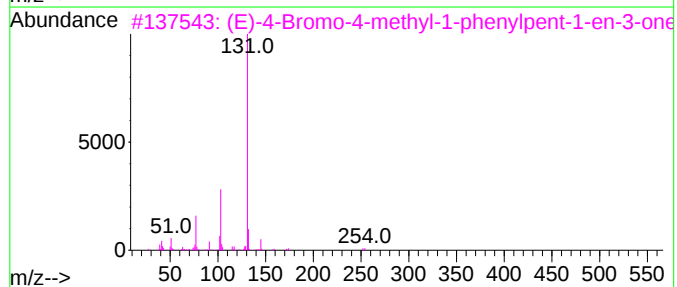
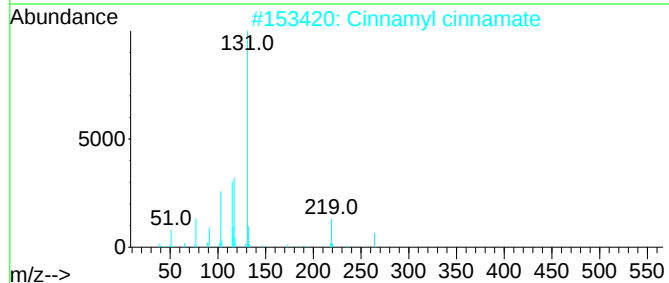
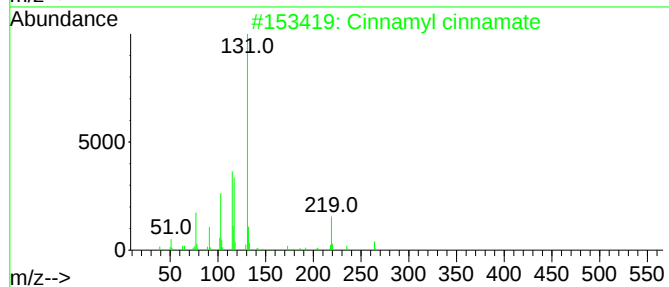
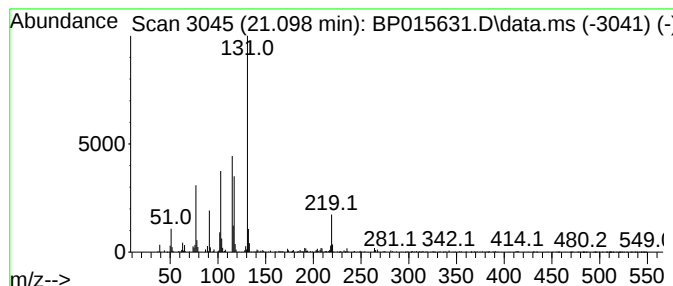
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Cinnamyl cinnamate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.098	2.81 ng/ul	316824	Chrysene-d12	21.569

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2			Cinnamyl cinnamate	264	C18H16O2	000122-69-0	72
3			(E)-4-Bromo-4-methyl-1-phenylpen...	252	C12H13BrO	1000443-02-8	50
4			Vinyl trans-cinnamate	174	C11H10O2	017719-70-9	49
5			N-(3-Chlorophenyl)-3-phenyl-2-pr...	271	C16H14ClNO	1507357-48-3	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062023\
Data File : BP015631.D
Acq On : 20 Jun 2023 20:26
Operator : MA/JU
Sample : 03080-20
Misc :
ALS Vial : 15 Sample Multiplier: 1

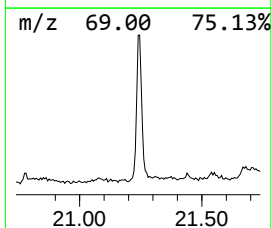
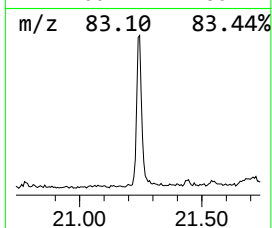
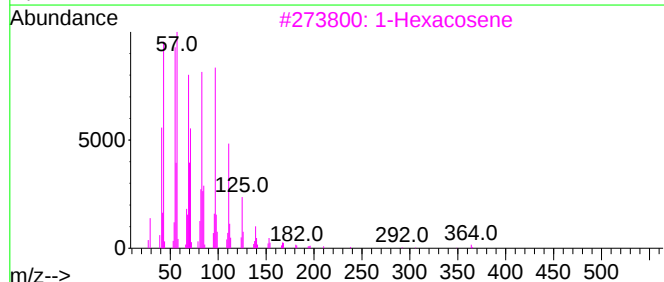
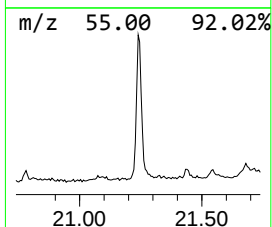
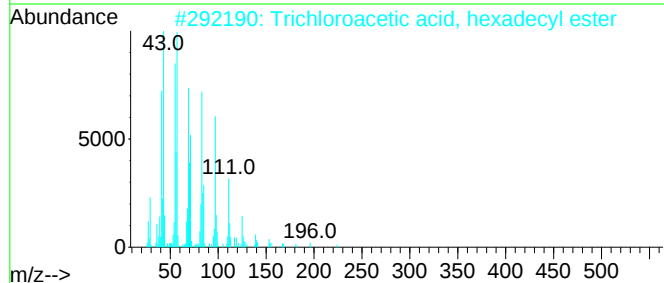
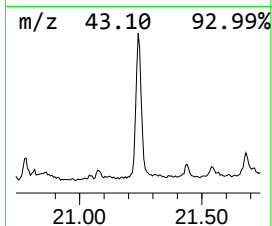
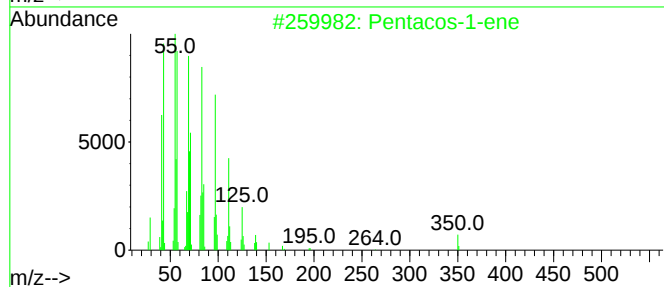
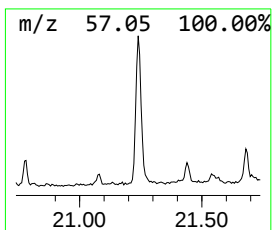
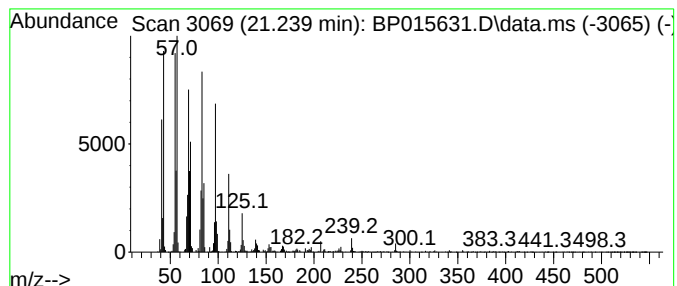
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BNA_P
ClientSampleId :
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.239	9.67 ng/ul	1089210	Chrysene-d12		21.569	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Pentacos-1-ene		350	C25H50	016980-85-1	94
2	Trichloroacetic acid, hexadecyl ...		386	C18H33Cl3O2	074339-54-1	94
3	1-Hexacosene		364	C26H52	018835-33-1	94
4	Nonacos-1-ene		406	C29H58	018835-35-3	94
5	1-Docosanethiol		342	C22H46S	007773-83-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062023\
Data File : BP015631.D
Acq On : 20 Jun 2023 20:26
Operator : MA/JU
Sample : 03080-20
Misc :
ALS Vial : 15 Sample Multiplier: 1

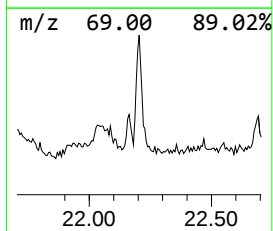
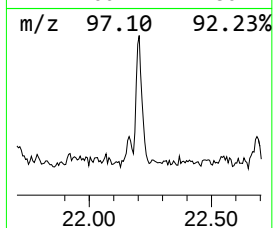
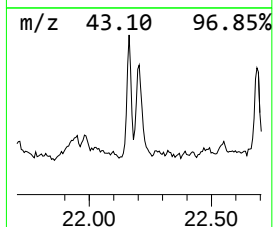
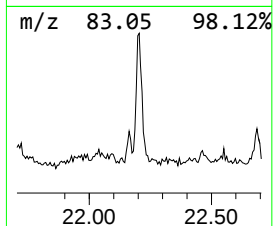
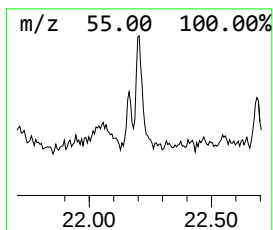
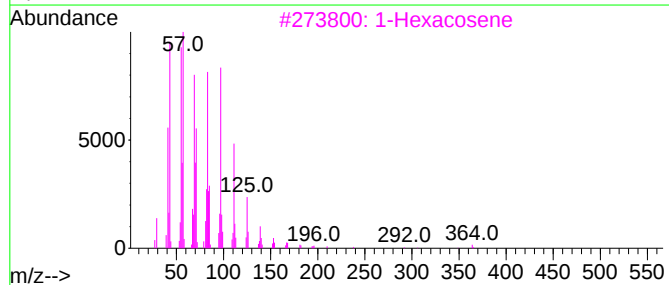
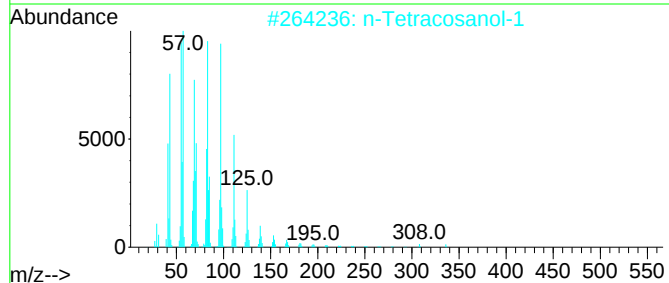
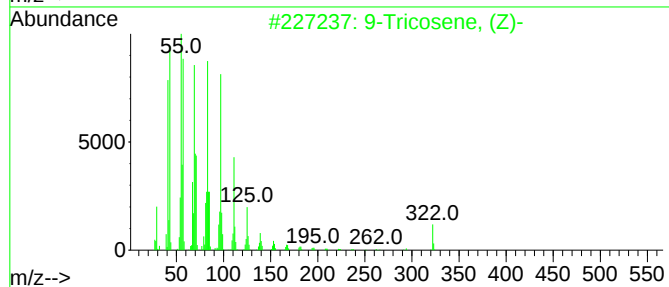
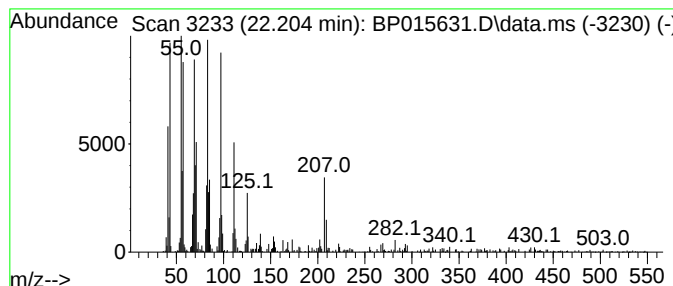
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
22.204	3.26 ng/ul	367395	Chrysene-d12		21.569	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	9-Tricosene, (Z)-		322	C23H46	027519-02-4	96
2	n-Tetracosanol-1		354	C24H50O	000506-51-4	94
3	1-Hexacosene		364	C26H52	018835-33-1	94
4	1-Heneicosanol		312	C21H44O	015594-90-8	94
5	Behenic alcohol		326	C22H46O	000661-19-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062023\
Data File : BP015631.D
Acq On : 20 Jun 2023 20:26
Operator : MA/JU
Sample : 03080-20
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFQ5

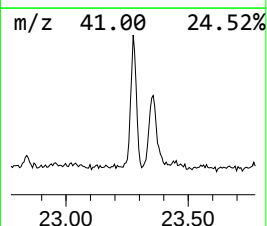
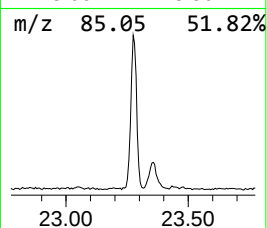
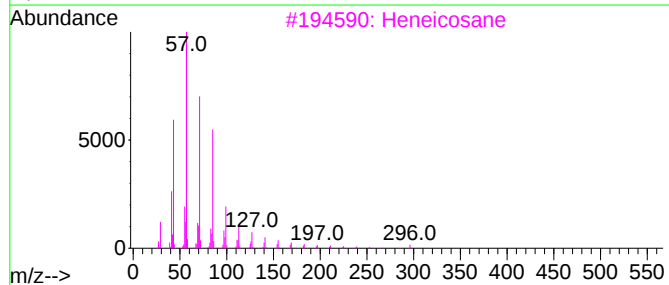
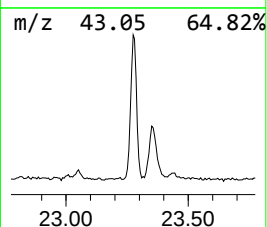
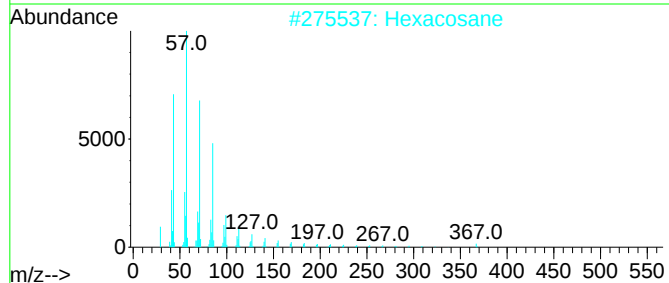
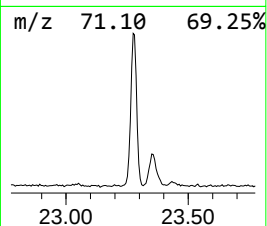
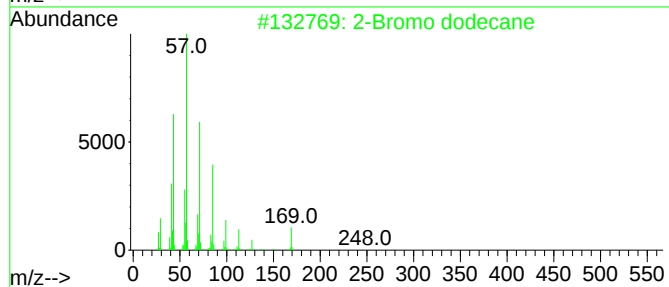
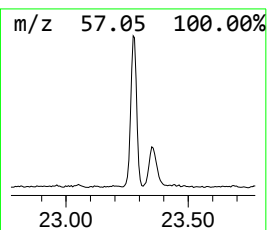
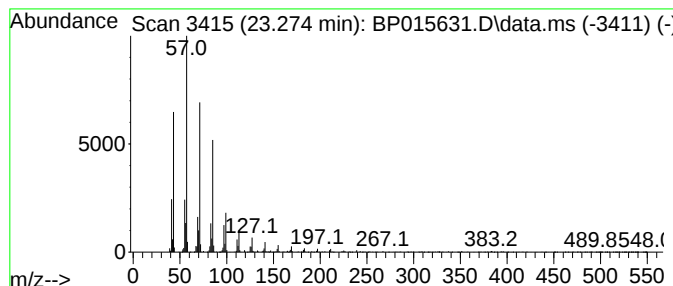
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 2-Bromo dodecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.274	9.43 ng/ul	1015520	Perylene-d12	24.116

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Bromo dodecane	248	C12H25Br	013187-99-0	93
2			Hexacosane	366	C26H54	000630-01-3	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062023\
Data File : BP015631.D
Acq On : 20 Jun 2023 20:26
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Sample : 03080-20
Misc :
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Instrument :
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ClientSampleId :
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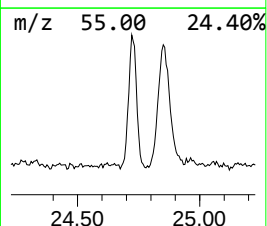
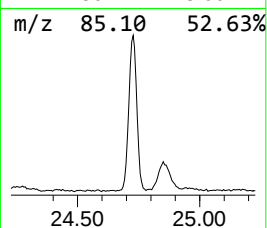
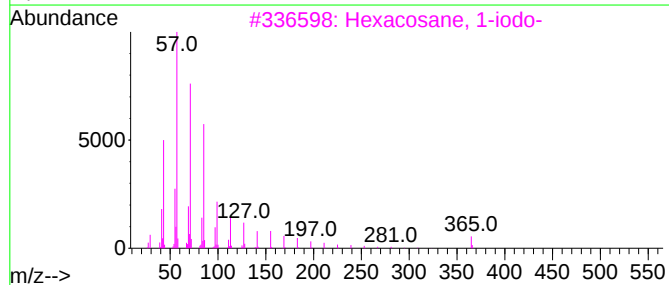
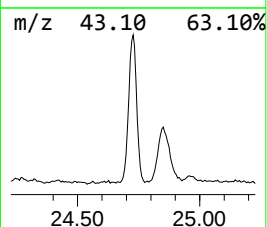
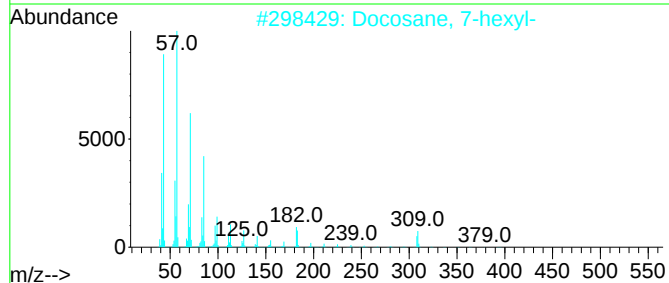
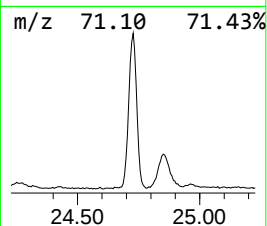
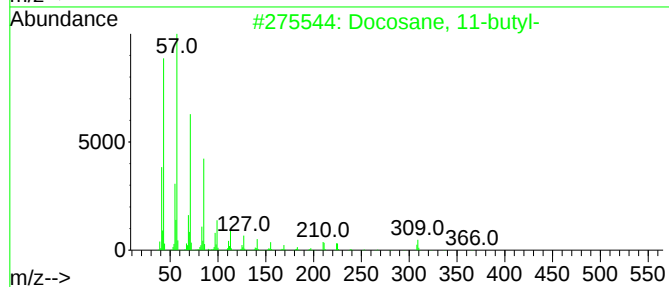
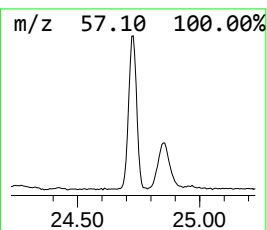
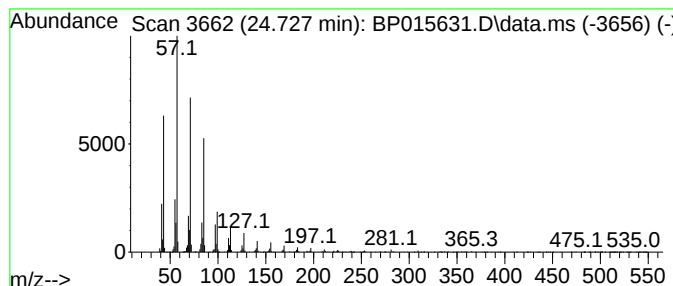
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.727	17.56 ng/ul	1891950	Perylene-d12	24.116

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosane, 11-butyl-	366	C26H54	013475-76-8	95
2			Docosane, 7-hexyl-	394	C28H58	055373-86-9	94
3			Hexacosane, 1-iodo-	492	C26H53I	1000406-32-1	91
4			Heneicosane	296	C21H44	000629-94-7	91
5			Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062023\
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ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzophenone	16.087	7.3	ng/ul	544978	3	14.728	1491530	20.0
n-Hexadecanoic ...	18.345	14.1	ng/ul	1446060	4	17.486	2044850	20.0
Octadecanoic acid	19.563	4.5	ng/ul	512949	5	21.569	2253590	20.0
Cinnamyl cinnamate	21.098	2.8	ng/ul	316824	5	21.569	2253590	20.0
(DEL) Alkane: S...	21.239	9.7	ng/ul	1089210	5	21.569	2253590	20.0
(DEL) Alkane: S...	22.204	3.3	ng/ul	367395	5	21.569	2253590	20.0
2-Bromo dodecane	23.274	9.4	ng/ul	1015520	6	24.116	2154640	20.0
(DEL) Alkane: S...	24.727	17.6	ng/ul	1891950	6	24.116	2154640	20.0